

NPS ARCHIVE
1964
TAYLOR, H.

Howard S. Taylor

RESONANT SCATTERING STATE OF
THE NEGATIVE HYDROGEN MOLECULE ION.

Thesis
T2213

Library**U. S. Naval Postgraduate School****Monterey, California**

Resonant Scattering State of the Negative
Hydrogen Molecule Ion.⁺

by

Howard S. Taylor*

and "

J. K. Williams**

Department of Chemistry
University of Southern California
Los Angeles, California 90007

Abstract

An ab-initio calculation is made on a resonant state of the H_2^- ion by an approximate variation method. Excellent agreement with experiment is obtained. Physical justification is given for the use of the approximate variation method.

-
- + Research supported by Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California.
- * Consultant to the Theoretical Chemistry Group at the Jet Propulsion Laboratory.
- ** Lieutenant, United States Navy, and participant in the Advanced Science (Chemistry) Postgraduate Education Program of the Navy.
-

IPS Archive

The¹³
~~T2~~ 213

1964

Taylor, H

I. Discussion

Several recent experiments have shown features that indicate the presence of an H_2^- ion. Schultz¹ proposed a state of H_2^- in the formation of H and H^- by electron impact on hydrogen gas. Khvostenko and Dukel'shii^{2a} proposed a similar mechanism in electron impact measurements on H_2 , i.e., $H_2 + e \rightarrow (H_2^-) \rightarrow H + H^-$. They also detected a negative ion of mass two by mass spectrometer^{2b} upon bombarding a mixture of water and antimony gas with electrons. In ref. (2b) is explained why this was felt to be H_2^- with a lifetime long enough to be observed, rather than the other possibility, D^- . In astrophysics³ it has been suggested that H_2^- occurs in the solar corona and dissociates into H and H^- .

The latest of these have been some electron scattering experiments by Simpson and Kuyatt,^{4,5} where a highly monochromatic electron beam was scattered off hydrogen gas. A plot of current vs. energy was made, and resonances corresponding to a set of vibrational levels were observed. From these levels the spectroscopic constants ω_e , $\omega_e x_e$, and the approximate E_0 were calculated. The spectroscopic constants are very similar to those of H_2 , $^1\Pi_u$ or $^3\Pi_u$, however the threshold energy was lower than both, thereby suggesting the possibility of a resonant state of H_2^- consisting roughly of an inner σ electron and two outer electrons, with symmetry $^2\Sigma_g^*$. (Note that the outermost, planetary electron would not greatly affect the field in which the nuclei move.)

The predominant common feature of all these experiments is that they are of a scattering nature, and thus the observations could be of a real bound excited state, or of a resonance in the continuum.

Previous papers concerning theoretical calculations⁶ on H_2^- show that there is no bound state with an energy lower than that of the $H_2 X \ ^1\Sigma_g$ state of the hydrogen molecule with an electron at infinity. In the computations of (6) many configurations were tried, with complete variation of non-linear and linear parameters, and in all cases the variation method itself produced the equivalent of a hydrogen molecule with an electron in the continuum.

Thus it was decided to look for a bound state of a different nature, i.e., following the suggestions of experiment, a state with one inner σ electron and two outer π electrons, such that essentially the wave function would resemble the trapping of an electron in a π orbital by a $^1\Pi_u$ or $^3\Pi_u$ hydrogen molecule. This appears physically reasonable since an incoming electron would "see" a σ electron about two nuclei, and a 1π electron perpendicular to it, or therefore,

* Σ^+ and Σ^- are essentially degenerate for this discussion. This can be seen from the small overlap of the (ξ, η) parts of 1π and 3π .

a net attractive charge which was greater than zero, since the excited orthogonal outer electron would not screen for the incoming one. Also, in both the two electron ($1\sigma\ 1\pi$) and the three electron ($1\sigma\ 1\pi\ 3\pi$) systems, the electrons are highly uncorrelated. The importance of this will be discussed later.

Note the difference between this and electron capture by a hydrogen atom to form H^- . In atoms an incoming electron can induce polarization, but in the hydrogen molecule, most of the electron density must remain between the two nuclei to form the bond, and therefore cannot be polarized nearly as much as two separate atoms by the incoming electron. This gives another physical picture of the reason a state like the $^1\Sigma_g$ state of hydrogen cannot capture an electron, but states like $^1\Pi_u$ and $^3\Pi_u$ might be likely to.

Use of a trial variation function of this type could lead to two possible results. First, but highly unlikely due to experimental evidence and previous theoretical calculations, there could be a true bound state which would be a solution to the Schrodinger equation, with a true variation principle and an energy less than that of the ground state of the hydrogen molecule. Or, secondly, the $1\sigma\ 1\pi$ configuration could cause a narrow, but very deep potential well for the incoming electron, such that there is a resonance, composed of a highly localized, relatively long-lived combination of continuum states (wave packet).

The problem then is to construct such a highly localized wave packet from continuum functions having a lifetime long enough to be observable. In other words, with a low probability of a radiationless transition from the resonant state to the hydrogen molecule plus an electron of proper energy in the continuum.

Using the physical arguments above, a configuration which will hopefully have a deep potential well for the scattered electron and a small overlap with the $H_2\ ^1\Sigma_g + e$ must be constructed. A preliminary calculation was made with a trial function with configuration $1\sigma 1\pi 1\pi$. Even this rough calculation confirmed the suspicion that there is no bound discrete state with an energy less than that of $H_2\ ^1\Sigma_g + e$. The second possibility then becomes the one which must be investigated. Certain difficulties arise, for there is no longer a variation theorem and no rigorous minimum principle. How does one select the parameters of a wave packet and calculate the energy under these circumstances? Two arguments will be given to show the validity of an approximate variation principle. They are based on the fact that the system is to a large degree uncorrelated, with weak interactions between electrons, and that the deep potential causes a resonance packet, which is a function of time, and this time dependence may, to

a first approximation, be expressed in the parameters of the trial function. Neither of these arguments can be proven rigorously, but the subsequent discussion and results show them both to be physically quite valid.

The variation principle requires that all bound states be orthogonal to all lower energy states of the same symmetry. In the present case, the packet approximating a bound state must be orthogonal to all ${}^2\Sigma_g^-$ state of $H_2^+ \Sigma_g^-$ plus an electron at infinity. Although rigorous orthogonality is impossible since both states are ${}^2\Sigma_g^-$, effective orthogonality (zero overlap) is possible if the packet is constructed so the two inner electrons are in $1s\sigma_g$, which is orthogonal to $H_2^+ \Sigma_g^-$. The variation is restricted such that the two inner electrons must remain in $1s\sigma_g$, i.e., $H_2^+ 1s\sigma_g$ and therefore are orthogonal to $H_2^+ \Sigma_g^-$. Orthogonality is also expected because the continuum electron in the lower state overlaps negligibly with the localized $1s\sigma_g$ packet. This has been verified by direct calculation of the overlap integrals of non-equal energy cases. If the packet were to overlap with any other state it would have to be those of equal energy. The following argument is presented to account for this case. It has been noticed in retrospect that good agreement with experiment, the insensitivity of the variation of one electron's parameters to the other's parameters, and the resulting well separated molecular orbitals indicate that the electron correlation is very small. If this is the case, $1/r_{12}$ can be considered as a perturbation and a zero order argument that the overlap is zero can be given. Higher order perturbation theory will give negligible overlap if there is "convergence" by zero order. If $\langle V_{corr.} \rangle$ is small then the configuration used is a product of three H_2^+ functions. The packet is $1s\sigma_g 1s\sigma_g^{-1} 3p\sigma_u^{-1}$; the continuum is $1s\sigma_g 1s\sigma_g^{-1} 3p\sigma_u^{-1}$ and these are clearly orthogonal by the orthogonality of H_2^+ orbitals. Therefore by perturbation theory, weak correlation implies that a restricted variation (restricted to different H_2^+ orbitals) allows a true minimum principle with which to calculate the "best" energy. To verify this it is noted in Holstein, and Pettett and Dahler's work on helium⁷ very reasonable results are obtained when the variation principle is applied to such uncorrelated packet states as $(2p)^2 {}^4F_g$, $(2p)^2 {}^2D_g$, $(2p3p) {}^1F_g$, $(2p3d) {}^1D_u$, and $(2p3d) {}^3D_u$. On the other hand Holstein finds that the $(2s)^2 {}^1S$ state^{7b} in H^- has a lower energy than that of the $(1s)^2 {}^1S$ state of H^- . In helium, the reverse, expected result is found. It is felt by the authors that the result on H^- is in error because in the $(2s)^2 {}^1S$ case correlation is not small and no approximate variation principle holds. Clearly $(2s)^2$

being lower than $(1s)^2$ is unphysical and contrary to the more extensive calculation of Pekeris^{8a} where he shows only one bound state exists. The $(2s)^2\ 1S$ problem in helium is also not completely settled.^{8a,b} This is felt to be due to the correlated nature of the system and the consequent failure of the variation method.

Another justification of the variation principle is that since this is a resonance, the energy calculated by variation is not a discrete eigenvalue, but the average of a spread of energies. This average energy must be a function of time, since the packet must eventually spread. Now there is no explicit time dependence in the variation function, but the variable parameters regulate the spread of the wave packet, and thus the parameters themselves may be considered as time dependent and tending to cause the resonant wave packet to delocalize as time increases.

To achieve the longest lived resonant state in the restricted region of Hilbert space selected, therefore, by the uncertainty principle, ΔE_{av} must be minimized.

This can be stated as $\bar{E}_{av} = E_{av}(\alpha_1)$, where α_1 are the variable parameters, and $\alpha_1 = \alpha_1(t)$. Then to minimize ΔE ,

$$\frac{\partial E_{av}}{\partial t} = 0 = \sum_i \frac{\partial E_{av}}{\partial \alpha_i} \frac{\partial \alpha_i}{\partial t} \quad (I.1)$$

But the variation method causes $\partial E_{av}/\partial \alpha_1 = 0$ for all α_1 therefore minimizing ΔE_{av} and maximizing Δt . This in essence selects the best (longest lifetime) wave packet possible in the region of Hilbert space considered. Note that the variation alone will not give a long lifetime state, but will only give the packet of longest lifetime among the class chosen.

The use of the variation principle has now been physically justified. Thus the question becomes: is the state which has been found of long enough lifetime to be observed? An appeal to the ultimate agreement with experiment could be made, with the claim that the state clearly exists long enough to vibrate. However, it is preferable to give a physical argument based on the weakness of the correlations and the resulting perturbation method to indicate a long lifetime.

To demonstrate this, consider the standard auto-ionization picture of bound states in the continuum.⁹ The argument will be outlined here for helium because it is easier; it will be clearly extendable to the H_2^- case. If

$1/r_{12} = V_{\text{corr.}}$ is small the zero order wave functions are products of two hydrogenic orbitals. The functions and levels fall into three classes with overlapping energies:

- (a) $E = -\frac{1}{n_1^2} - \frac{1}{n_2^2}$ both one-electron functions bound
- (b) $E = -\frac{1}{n_1^2} + \frac{k_2^2}{2}$ one one-electron function bound and one continuum
- (c) $E = \frac{k_1^2}{2} + \frac{k_2^2}{2}$ both continuum

When n_1 and n_2 are large in (a) and n_1 small in (b), a k can be found such that $E_{\text{cont.}} = E_{\text{bd.}}$, i.e., there exists a bound state in the continuum. A non-radiative transition from the bound to continuum state of equal energy is given by the probability of auto-ionization (see ref. 9, and ref. 7a). Therefore the transition probability, w , is proportional to

$$\left| \langle \text{bound} \left| \frac{1}{r_{12}} \right| \text{cont.} \rangle \right|^2 \delta(E_{\text{bd.}} - E_{\text{cont.}})$$

The lifetime of the bound state is proportional to w^{-1} .

Now if the correlation is small, an assumption upon which the equation for w was derived, the first order correction to the bound state function due to correlation is given by

$$(H_0 - E_{\text{bd.}}) \psi_1 + \left(\frac{1}{r_{12}} - E_1 \right) \psi_{\text{bd.}} = 0$$

If ψ_1 is expanded as usual on all other states of the system, and substituted back into the perturbation equation, then multiplied by $\psi_{\text{cont.}}$ and integrated, the result is,*

$$\langle \text{bound} \left| \frac{1}{r_{12}} \right| \text{cont.} \rangle + C_{\text{bd. on cont.}} (E_{\text{bd.}} - E_{\text{cont.}}) = 0$$

Now when $E_{\text{bd.}} = E_{\text{cont.}}$ the matrix element is to first order zero and w is then of the form $x\delta(x)$, $x = E_{\text{bd.}} - E_{\text{cont.}}$, and therefore approximately zero. Higher order perturbation theory modifies this, but if the perturbation is really small, in a negligible way.

In support of this argument it is pointed out that the types of resonant states that have been observed are generally highly uncorrelated and ones in which the "resonant trapped" electron sees a deep well due to the rest of the system. It is exactly this type of state for which successful variation calculations have been carried out.

* In this expression, the continuum normalization factors have been cancelled from both sides.

II. Wave Function and Calculation Methods

Using the physical arguments above, it was decided to use a one configuration three-electron variation function, having ${}^2\Sigma_g$ symmetry, such that loss of the outer electron would not be able to yield a ${}^1\Sigma_g$ state, but only a ${}^1\Pi_u$ state. The elliptic molecular orbitals and calculation methods of Harris and Taylor were used.¹⁰

For one configuration the variation function becomes:

$$\Psi^d(\bar{r}, \bar{\sigma}) = 6^{-\frac{1}{2}} \sum_{j=1}^2 \sum_P U_{jd}(P) \Phi(P\bar{r}) \Theta_{\lambda_j}^3(\bar{\sigma}) \quad (\text{II.1})$$

where $U_{jd}(P)$ is the jd element of the matrix representation of the permutation P on the spin eigenfunction bases. The $\Theta_{\lambda_j}^3$ are:¹¹

$$\begin{aligned} \Theta_{\lambda_{j01}}^3(\bar{\sigma}) &= 6^{-\frac{1}{2}} (2\alpha\alpha\beta - \alpha\beta\alpha - \beta\alpha\alpha) \\ \Theta_{\lambda_{j02}}^3(\bar{\sigma}) &= 2^{-\frac{1}{2}} (\alpha\beta\alpha - \beta\alpha\alpha) \end{aligned} \quad (\text{II.2})$$

The spatial part is the product,

$$\chi(\bar{r}) = \prod_{i=1}^3 \phi_i(\bar{r}_i) + \prod_{i=1}^3 \phi'_i(\bar{r}_i) \quad (\text{II.3})$$

where the ϕ_i are of the form,

$$\phi_i(\delta_i, \alpha_i; n, m, v) = \exp[-(\delta_i \xi_i + \alpha_i \eta_i + i v \phi_i)] \xi_i^{n_i} \eta_i^{m_i} [(\xi_i^2 - 1)(1 - \eta_i^2)]^{\frac{|v_i|}{2}} \quad (\text{II.4})$$

and the ϕ_i' are,

$$(-1)^{m_i + |v_i|} \phi_i(\delta_i, -\alpha_i; n, m, v) \quad (\text{II.5})$$

ξ , η and ϕ being the standard two-center elliptical coordinates. The δ_i , α_i are variable within the computer program used, but n, m, v are input parameters and therefore fixed throughout the problem. The configuration chosen was:

$$\phi_1(\delta_1, \alpha_1; 0, 0, 0) \phi_2(\delta_2, \alpha_2; 0, 0, 1) \phi_3(\delta_3, \alpha_3; 2, 0, -1) + \phi'_1 \phi'_2 \phi'_3 \quad (\text{II.6})$$

It is convenient to denote these in terms of the v_i , since none of the n, m, v change and all $m_i = 0$. Thus,

$$\chi(\bar{r}) = \phi_0 \phi_1 \phi_{-1} + \phi'_0 \phi'_1 \phi'_{-1} \quad (\text{II.7})$$

Since $\Sigma m_i = 0$ and $\Sigma |v_i| = 2$, there is no sign change between the products, and gerade symmetry is ensured. Also, $\Sigma v_i = 0$, so the three electron product is a Σ state.

Note that if the outer electron is removed (placed in the continuum),

$$\chi(\bar{r}) = [\phi_0 \phi_1 + \phi'_0 \phi'_1] \phi(3) \quad (\text{II.8})$$

is obtained, which is a Π state ($\Sigma v \neq 0$) with ungerade symmetry since the ϕ_1'

introduces a - sign between the products. Thus it has been spatially ensured that the 1 configuration variation function cannot vary itself to $H_2 \ ^1\Sigma_g + e$ by varying δ_{-1} to a very small number which has the effect of ejecting the outer electron into the continuum.

Looking at the spin portion, it is also noted that $\Theta_{\chi\sigma 1}^3$ can "lose" an electron to become,

$$\Theta_{\infty 1}^2 \chi(3) = 2^{-1/2} [(\alpha\beta - \beta\alpha)] \chi(3) \quad (\text{II.9})$$

which is the spin eigenfunction for a two electron singlet.

The one-configuration variation function is now constrained in such a manner that it cannot eject the outer electron and become anything but $H_2 \ ^1\Pi_u + e$, and the resonant wave packet is suitably localized by these constraints.

III. Calculations and Results

In order to obtain a potential curve and the spectroscopic constants for comparison with those reported by experiment,⁴ it was planned to calculate five energy values at nuclear radii corresponding to scaled roots of the fifth order Chebyshev polynomial $T_5(x)$, where $x = (R - R_e)/.34026$, which gives separations of $\pm .2000$ and $\pm .3236$ au. about R_e , and fit these to Chebyshev polynomials T_0 through T_4 .¹² The spectroscopic constants could then be calculated by the method of Dunham.¹³

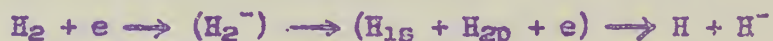
Preliminary calculations with a trial function of the type $1\sigma(1\pi)^2$ yielded an equilibrium radius of 1.9196 au., and the final full variation of the δ and α parameters was done about this R_e . Upon fitting to the Chebyshev polynomials and minimizing $E(R)$ with respect to R , R_e was found to be 1.949 au. instead of 1.9196, so Dunham's method, based on a polynomial in $(R - R_e)/R_e$, becomes excessively tedious. Therefore, the polynomial in x was converted to a polynomial in R and the vibration-rotation constants calculated by the method used by Fraga and Ransil in ref. 14.

To note the effect of greater interatomic distances three other R values were used. Table I gives the potential curve and parameters of the wave function.

Table II is a comparison of the calculated spectroscopic constants with those reported in the scattering experiment.

It is also of interest to note in Table III that as R increases, the potential curve approaches the curve of the $^1\Pi_u$ state of H_2 .¹⁵ This can be explained by inspection of the parameters of the three electrons. At $R = 10.0$ au. there is essentially a 1s hydrogen atom and a 1p hydrogen atom widely separated, with an electron in between. In H_2 $^1\Pi_u$ at this internuclear distance, the expected configuration is a pair of hydrogen atoms, one in the 1s state and one in the 1p state.

This seems to indicate that H_2^- cannot be formed by collision of H and H^- , but only by collision of H_2 with an electron. Also, the proposed mechanism for formation of H and H^- by dissociation of H_2^- may have another step,



where the H_{2p} may recapture the electron of the H_2^- or capture another of the electrons in the experimental system.

IV. Conclusions

The potential curve and electronic wave function for the resonant $^2\Sigma_g$ state of H_2^- have been calculated by treating a one-configuration trial function as if it were a real variation function which could be minimized to a real discrete eigenvalue. An average energy very near to the experimentally observed energy was obtained, however, since this is a state in the continuum there is no rigorous minimum principle, and the calculated average energy may be above or below the actual energy of the system.

There is no doubt that if the configuration determining parameters n , m , and v were also allowed to vary, the final result would have been the one configuration approximation to the ground state energy of the hydrogen molecule.

Excellent agreement with experimental spectroscopic constants has been obtained, which substantiates the statement that this is a resonance with a lifetime long enough to be observable, and the use of physical intuition to pick a restricted variation function which simulates an electron scattering off a deep, narrow potential well formed by an excited state of H_2 .

The method of finding the longest-lived wave packet in the continuum by a restricted variation method coupled with good physical guesses may have considerable application in other problems.

It is the intuitive feeling of the authors that all resonant states will be able to be treated by this approximate method, because if they have a long enough lifetime to be observed, they are probably weakly correlated, in the sense described above and therefore amenable to approximate variation treatment. This may not be a necessary condition, but it is certainly a sufficient one. The lack of rigor prescribes great care in any application.

V. Acknowledgment

The authors would like to acknowledge useful discussions with Dr. M. Saffrin of the Jet Propulsion Laboratory, and Professor M. H. L. Pryce of the Physics Department of the University of Southern California.

Table I^a

Wave Function and Potential Curve

R (au)	-E (au)	δ	α	R (au)	-E (au)	δ	α
1.596	.74336	1.115	.765	2.2432	.74488	1.420	1.020
		.445	-.17			.635	-.255
		.100	0.0			.105	0.0
1.7196	.74848	1.175	.810	3.000	.71513	1.75	1.34
		.485	-.185			.82	-.38
		.105	0.0			.11	0.0
1.9196	.75064	1.270	.890	7.000	.63377	3.53	3.39
		.550	-.210			1.78	-1.66
		.105	0.0			.11	0.0
2.1196	.74804	1.365	.970	10.000	.62929	5.01	4.96
		.600	-.240			2.51	-2.50
		.105	0.0			.11	0.0
				15.00 ^b	.61332	6.24	6.21
						3.76	-3.76
						.10	0.0

- a. Throughout this table, the electron parameters are listed in the order $\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 2 & 0 & -1 \end{pmatrix}$ so that the inner electron is first, and

the outer resonant electron is last.

- b. This point was not completely varied, but a definite continuation of the trend to $H_{1s} + H_{1p} + e^-$ is exhibited.

Table 1

Mean values of the variables

		Age	Sex	Height	Weight	Body mass index	Body fat
1	10-14	10-14	Male	140	35	25.0	15.0
2	15-19	15-19	Male	160	55	34.4	18.0
3	20-24	20-24	Male	170	75	41.2	20.0
4	25-29	25-29	Male	175	85	43.5	22.0
5	30-34	30-34	Male	178	90	45.5	23.0
6	35-39	35-39	Male	180	95	47.2	24.0
7	40-44	40-44	Male	182	100	49.5	25.0
8	45-49	45-49	Male	185	105	51.9	26.0
9	50-54	50-54	Male	188	110	54.3	27.0
10	55-59	55-59	Male	190	115	56.3	28.0
11	60-64	60-64	Male	192	120	58.3	29.0
12	65-69	65-69	Male	195	125	60.0	30.0
13	70-74	70-74	Male	198	130	61.1	31.0
14	75-79	75-79	Male	200	135	62.5	32.0
15	80-84	80-84	Male	202	140	64.4	33.0
16	85-89	85-89	Male	205	145	66.3	34.0
17	90-94	90-94	Male	208	150	68.3	35.0
18	95-99	95-99	Male	210	155	70.0	36.0
19	100-104	100-104	Male	212	160	72.6	37.0
20	105-109	105-109	Male	215	165	74.4	38.0
21	110-114	110-114	Male	218	170	76.6	39.0
22	115-119	115-119	Male	220	175	78.2	40.0
23	120-124	120-124	Male	222	180	80.0	41.0
24	125-129	125-129	Male	225	185	81.8	42.0
25	130-134	130-134	Male	228	190	83.3	43.0
26	135-139	135-139	Male	230	195	85.0	44.0
27	140-144	140-144	Male	232	200	86.2	45.0
28	145-149	145-149	Male	235	205	87.7	46.0
29	150-154	150-154	Male	238	210	88.7	47.0
30	155-159	155-159	Male	240	215	90.0	48.0
31	160-164	160-164	Male	242	220	91.3	49.0
32	165-169	165-169	Male	245	225	92.2	50.0
33	170-174	170-174	Male	248	230	93.1	51.0
34	175-179	175-179	Male	250	235	94.0	52.0
35	180-184	180-184	Male	252	240	95.2	53.0
36	185-189	185-189	Male	255	245	96.1	54.0
37	190-194	190-194	Male	258	250	97.3	55.0
38	195-199	195-199	Male	260	255	98.1	56.0
39	200-204	200-204	Male	262	260	99.2	57.0
40	205-209	205-209	Male	265	265	100.0	58.0
41	210-214	210-214	Male	268	270	101.1	59.0
42	215-219	215-219	Male	270	275	101.9	60.0
43	220-224	220-224	Male	272	280	102.9	61.0
44	225-229	225-229	Male	275	285	103.7	62.0
45	230-234	230-234	Male	278	290	104.7	63.0
46	235-239	235-239	Male	280	295	105.4	64.0
47	240-244	240-244	Male	282	300	106.4	65.0
48	245-249	245-249	Male	285	305	107.4	66.0
49	250-254	250-254	Male	288	310	108.3	67.0
50	255-259	255-259	Male	290	315	109.0	68.0
51	260-264	260-264	Male	292	320	110.0	69.0
52	265-269	265-269	Male	295	325	110.9	70.0
53	270-274	270-274	Male	298	330	111.8	71.0
54	275-279	275-279	Male	300	335	112.5	72.0
55	280-284	280-284	Male	302	340	113.6	73.0
56	285-289	285-289	Male	305	345	114.4	74.0
57	290-294	290-294	Male	308	350	115.3	75.0
58	295-299	295-299	Male	310	355	116.1	76.0
59	300-304	300-304	Male	312	360	117.0	77.0
60	305-309	305-309	Male	315	365	117.8	78.0
61	310-314	310-314	Male	318	370	118.9	79.0
62	315-319	315-319	Male	320	375	119.7	80.0
63	320-324	320-324	Male	322	380	120.8	81.0
64	325-329	325-329	Male	325	385	121.6	82.0
65	330-334	330-334	Male	328	390	122.6	83.0
66	335-339	335-339	Male	330	395	123.3	84.0
67	340-344	340-344	Male	332	400	124.4	85.0
68	345-349	345-349	Male	335	405	125.1	86.0
69	350-354	350-354	Male	338	410	126.1	87.0
70	355-359	355-359	Male	340	415	126.8	88.0
71	360-364	360-364	Male	342	420	127.8	89.0
72	365-369	365-369	Male	345	425	128.4	90.0
73	370-374	370-374	Male	348	430	129.3	91.0
74	375-379	375-379	Male	350	435	130.0	92.0
75	380-384	380-384	Male	352	440	131.0	93.0
76	385-389	385-389	Male	355	445	131.8	94.0
77	390-394	390-394	Male	358	450	132.7	95.0
78	395-399	395-399	Male	360	455	133.3	96.0
79	400-404	400-404	Male	362	460	134.3	97.0
80	405-409	405-409	Male	365	465	135.1	98.0
81	410-414	410-414	Male	368	470	136.1	99.0
82	415-419	415-419	Male	370	475	136.8	100.0
83	420-424	420-424	Male	372	480	137.8	101.0
84	425-429	425-429	Male	375	485	138.4	102.0
85	430-434	430-434	Male	378	490	139.4	103.0
86	435-439	435-439	Male	380	495	140.0	104.0
87	440-444	440-444	Male	382	500	141.1	105.0
88	445-449	445-449	Male	385	505	141.8	106.0
89	450-454	450-454	Male	388	510	142.8	107.0
90	455-459	455-459	Male	390	515	143.3	108.0
91	460-464	460-464	Male	392	520	144.4	109.0
92	465-469	465-469	Male	395	525	145.1	110.0
93	470-474	470-474	Male	398	530	146.2	111.0
94	475-479	475-479	Male	400	535	146.8	112.0
95	480-484	480-484	Male	402	540	147.9	113.0
96	485-489	485-489	Male	405	545	148.4	114.0
97	490-494	490-494	Male	408	550	149.5	115.0
98	495-499	495-499	Male	410	555	150.0	116.0
99	500-504	500-504	Male	412	560	151.0	117.0
100	505-509	505-509	Male	415	565	151.8	118.0
101	510-514	510-514	Male	418	570	152.9	119.0
102	515-519	515-519	Male	420	575	153.6	120.0
103	520-524	520-524	Male	422	580	154.7	121.0
104	525-529	525-529	Male	425	585	155.3	122.0
105	530-534	530-534	Male	428	590	156.3	123.0
106	535-539	535-539	Male	430	595	156.8	124.0
107	540-544	540-544	Male	432	600	157.9	125.0
108	545-549	545-549	Male	435	605	158.4	126.0
109	550-554	550-554	Male	438	610	159.4	127.0
110	555-559	555-559	Male	440	615	160.0	128.0
111	560-564	560-564	Male	442	620	161.1	129.0
112	565-569	565-569	Male	445	625	161.8	130.0
113	570-574	570-574	Male	448	630	162.9	131.0
114	575-579	575-579	Male	450	635	163.3	132.0
115	580-584	580-584	Male	452	640	164.4	133.0
116	585-589	585-589	Male	455	645	165.1	134.0
117	590-594	590-594	Male	458	650	166.2	135.0
118	595-599	595-599	Male	460	655	166.8	136.0
119	600-604	600-604	Male	462	660	167.9	137.0
120	605-609	605-609	Male	465	665	168.4	138.0
121	610-614	610-614	Male	468	670	169.5	139.0
122	615-619	615-619	Male	470	675	170.0	140.0
123	620-624	620-624	Male	472	680	171.1	141.0
124	625-629	625-629	Male	475	685	171.8	142.0
125	630-634	630-634	Male	478	690	172.9	143.0
126	635-639	635-639	Male	480	695	173.3	144.0
127	640-644	640-644	Male	482	700	174.4	145.0
128	645-649	645-649	Male	485	705	175.1	146.0
129	650-654	650-654	Male	488	710	176.2	147.0
130	655-659	655-659	Male	490	715	176.8	148.0
131	660-664	660-664	Male	492	720	177.9	149.0
132	665-669	665-669	Male	495	725	178.4	150.0
133	670-674	670-674	Male	498	730	179.5	151.0
134	675-679	675-679	Male	500	735	180.0	152.0
135	680-684	680-684	Male	502	740	181.1	153.0
136	685-689	685-689	Male	505	745	181.8	154.0
137	690-694	690-694	Male	508	750	182.9	155.0
138	695-699	695-699	Male	510	755	183.3	156.0
139	700-704	700-704	Male	512	760	184.4	157.0
140	705-709	705-709	Male	515	765	185.1	158.0
141	710-714	710-714	Male	518	770	186.2	159.0
142	715-719	715-719	Male	520	775	186.8	160.0
143	720-724	720-724	Male	522	780	187.9	161.0
144	725-729	725-729	Male	525	785	188.4	162.0
145	730-734	730-734	Male	528	790	189.5	163.0
146	735-739	735-739	Male	530	795	190.0	164.0
147	740-744	740-744	Male	532	800	191.1	165.0
148	745-749	745-749	Male	535	805	191.8	166.0
149	750-754	750-754	Male	538	810	192.9	167.0
150	755-759	755-759	Male	540	815	193.3	168.0
151	760-764	760-764	Male	542	820	194.4	169.0
152	765-769	765-769	Male	545	825	195.1	170.0
153	770-774	770-774	Male	548	830	196.2	171.0
154	775-779	775-779	Male	550	835	196.8	172.0
155	780-784	780-784	Male	552	840	197.9	173.0
156	785-789	785-789	Male	555	845	198.4	174.0
157	790-794	790-794	Male				

Table II
Comparison of Spectroscopic Constants

	calculated	experimental
E	$-.75148 \text{ au}$	$-.738 \text{ au}$
R_e	1.949 au	
ω_e	$.30 \text{ ev}$	$.31 \text{ ev}$
ω_{e^*e}	$.042 \text{ ev}$	$\sim .01 \text{ ev}$
B_e	$.0039 \text{ ev}$	
α_e	$3 \times 10^{-4} \text{ ev}$	
D_e	5.36 ev	

Table III

Comparison with H_2 $^1\Pi_u$ Potential Curve

R (au)	$-E_{H_2C} \ ^1\Pi_u^a$	$-E_{H_2} \ ^2\Sigma_g$	ΔE
1.9	.71422	.75057	.03635
2.0	.71418	.74800	.03382
2.25	.71006	.74481	.03475
3.0	.68445	.71513	.03068
7.0	.62478	.63377	.00899
10.0	.62448	.62929	.00481

a. From ref. (12)

July 1975

Water Quality Data of the Colorado River

Station	Flow (cfs)	Temperature (°F)	Dissolved Oxygen (ppm)
1	100	72	8.5
2	150	73	8.2
3	200	74	8.0
4	250	75	7.8
5	300	76	7.5
6	350	77	7.2
7	400	78	7.0
8	450	79	6.8
9	500	80	6.5
10	550	81	6.2
11	600	82	6.0
12	650	83	5.8
13	700	84	5.5
14	750	85	5.2
15	800	86	5.0
16	850	87	4.8
17	900	88	4.5
18	950	89	4.2
19	1000	90	4.0
20	1050	91	3.8
21	1100	92	3.5
22	1150	93	3.2
23	1200	94	3.0
24	1250	95	2.8
25	1300	96	2.5
26	1350	97	2.2
27	1400	98	2.0
28	1450	99	1.8
29	1500	100	1.5
30	1550	101	1.2
31	1600	102	1.0
32	1650	103	0.8
33	1700	104	0.5
34	1750	105	0.2
35	1800	106	0.0

Continued on page 2

References

1. G. J. Schulz, Phys. Rev., 113, 816 (1959).
2. (a) V. I. Khvostenko and V. M. Dukel'shii, Soviet Physics JETP, 6, 657 (1957).
(b) V. I. Khvostenko and V. M. Dukel'shii, Soviet Physics JETP, 7, 709 (1958).
3. Y. Ūhman, Arkiv, Astron., 2, 1 (1955).
4. A. Ben-Reuven (private communication). C. E. Kuyatt, S. R. Mielczarek, and J. A. Simpson, Phys. Rev. Letters, 12, 293 (1964). U. Fano and J. W. Cooper, Paper HALO at Philadelphia Am. Phys. Soc. meeting, March 25, 1964 (not published).
5. For a description of the experimental technique see the articles by J. Arol Simpson in Proc. of the 3rd Int. Symposium in Atomic and Molecular Collisions (North-Holland Pub. Co., New Amsterdam, 1964). Also J. A. Simpson and U. Fano, Phys. Rev. Ltrs., 11, 158 (1963).
6. H. S. Taylor and F. E. Harris, J. Chem. Phys., 39, 1012 (1963). H. S. Taylor and John Gerhauser, J. Chem. Phys., 40, 244 (1964). The Taylor-Harris paper includes a critical review of previous theoretical calculations on H_2^+ .
7. (a) E. Holøien, Phys. Norvegica, 1, 53 (1961). E. Holøien, Phys. Rev., 104, 1301 (1956).
(b) E. Holøien, Proc. Phys. Soc., A71, 357 (1958). E. Holøien, Proc. Phys. Soc., A72, 141 (1958).
(c) P. M. Becker and J. C. Dahler, Phys. Rev., 136, A73 (1964).
8. (a) C. L. Pekeris, Phys. Rev., 126, 1470 (1962).
(b) B. F. Gray and H. O. Pritchard, J. Chem. Phys., 28, 519 (1958).
9. G. Herzberg, "Spectra of Diatomic Molecules," Chap. VII (D. Van Nostrand and Co., New York, 1950).
10. F. E. Harris, J. Chem. Phys., 32, 3 (1960). H. S. Taylor and F. E. Harris, Mol. Phys., 6, 183 (1963).
11. M. Kotani, "Table of Molecular Integrals" (Maruzen Co. Ltd., Tokyo, Japan, 1955).
12. R. K. Nesbet, J. Chem. Phys., 40, 3619 (1964).
13. J. L. Dunham, Phys. Rev., 41, 721 (1932).
14. S. Fraga and B. J. Ransil, J. Chem. Phys., 35, 669 (1961).
15. J. C. Browne, J. Chem. Phys., 40, 43 (1964).

My dear Mr. [Name]

I have just received your letter of the 15th inst. and am glad to hear that you are well and happy.

I am writing you a few lines to let you know that I am still in the same old place.

I have been thinking of you very much lately and wondering how you are getting on.

I hope you are still as healthy and happy as ever.

I have been very busy lately but I have managed to find some time to write you.

I have been thinking of you very much lately and wondering how you are getting on.

I hope you are still as healthy and happy as ever.

I have been very busy lately but I have managed to find some time to write you.

I have been thinking of you very much lately and wondering how you are getting on.

I hope you are still as healthy and happy as ever.

I have been very busy lately but I have managed to find some time to write you.

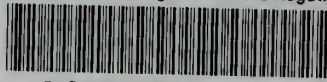
I have been thinking of you very much lately and wondering how you are getting on.

I hope you are still as healthy and happy as ever.

I have been very busy lately but I have managed to find some time to write you.

thesT2213

Resonant scattering state of the negativ



3 2768 002 03398 7

DUDLEY KNOX LIBRARY